Juliane Müller
Lawrence Berkeley National Laboratory
Center for Computational Sciences and Engineering
Berkeley, CA, 94720, USA
julianemueller@lbl.gov
(+1) 607-280-3868

Research Interests

I am interested in numerical optimization, in particular, I focus on black-box optimization problems whose objective and constraint function evaluations are based on a computationally expensive computer simulation. Previously, I developed efficient derivative-free algorithms for optimization problems with continuous, integer, and mixed-integer variables and that may have multiple computationally expensive black-box objective and constraint functions that may fail to evaluate (hidden constraints). I use surrogate models (response surface models) in order to cheaply approximate and predict the behavior of the expensive simulation functions. In the course of my research I addressed applications arising in vehicle routing, transportation network design, structural optimization, optimal reliability design, airfoil design, renewable energy (hydropower, kite energy), watershed management, groundwater remediation, global climate models, and combustion model calibration. Recently, I also started an effort that focuses on developing data-driven models for predicting groundwater levels in California, USA.

Education

Ph.D. in Applied Mathematics 09/2008 - 12/2012

School: Tampere University of Technology, Department of Mathematics, Tampere, Finland
Project: Surrogate Model Algorithms for Computationally Expensive Black-Box Global Optimization Problems
Advisor: Robert Piché

Visiting Ph.D. student in Applied Mathematics 11/2010 - 03/2012

School: Cornell University, Center of Applied Mathematics, Ithaca, NY, USA
Advisor: Christine A. Shoemaker

Diploma in Applied Mathematics (equivalent to Master of Science) 10/2003 - 06/2008

School: Technical University Bergakademie Freiberg, Germany
Project: Algorithms for the Bicriterion Vehicle Routing Problem with Time Windows
Advisors: Prof. Stephan Dempe (Technical University Bergakademie Freiberg), Risto Silvennoinen (Tampere University of Technology)

Research Experience

Research Scientist 05/2017 - current
Organization: Lawrence Berkeley National Laboratory, Center for Computational Sciences and Engineering, Berkeley, CA, USA
Research focus is on the development of efficient optimization algorithms and their application to various science problems including cosmology, combustion, high energy physics, and earth sciences.

Luis W. Alvarez Postdoctoral Fellow 08/2014 - 05/2017

Organization: Lawrence Berkeley National Laboratory, Center for Computational Sciences and Engineering, Berkeley, CA, USA
Research focus was on the development of new algorithms for solving computationally expensive black-box optimization problems

Postdoctoral Associate 01/2013 - 07/2014

School: Cornell University, School of Civil and Environmental Engineering, Ithaca, NY, USA
Project 1: Optimization algorithm development for the calibration of global climate models
Project 2: Optimization algorithm development for transportation network design problems

Internship 06/2008 - 08/2008

Organization: Finland Futures Research Center, Tampere, Finland
Project: Data analysis and forecasts related to the sustainable development of EU countries

Academic Service Experience

Member of the advisory board of study affairs at Technical University Bergakademie Freiberg, Department of Mathematics, Germany, 10/2005 - 04/2007

Tutor for incoming international students at Tampere University of Technology, academic year 2009-2010

Teaching Experience

Course Instructor

At Tampere University of Technology: Optimization Theory I: linear and nonlinear programming, teaching via video conferencing (lectures and recitation classes, participants ranged from pre-Bachelor to Ph.D. students), Fall 2011 - Spring 2012 while at Cornell University

At Cornell University: Interim instructor for special topics course on surrogate-based optimization for Ph.D. students, Spring 2014

Teaching Assistant at Tampere University of Technology

Stochastic Processes (recitation classes, course for postgraduate and graduate students), Fall 2010

Matrix Algebra 2 (assignment grading, course for graduate and postgraduate students), Spring 2010

Numerical Analysis (recitation classes, PC labs, course for undergraduate and graduate students), Spring 2010

Introduction to optimal design (recitation classes for international students, course for undergraduate and graduate students), Fall 2008

Relevant Courses and Workshops

Workshop on "The Essential Steps to Leadership", LBNL, June 27, 2017

Workshop on "Empathy: A Building Block for Inclusiveness", LBNL, January 10, 2017

Scientific Leadership and Management Skills Course, University of California, San Francisco, CA, USA, May 2016, certificate of participation

Teaching Workshops at Cornell University 10/2013 - 04/2014:

GET SET workshop series *"Building Mentoring Skills for a Career in Academia"*

University-Wide GET SET Teaching Conference (certificate, March 1, 2014)

GET SET workshop series (certificates in *"Enhancing Teaching with Technology"* and *"Creating an Engaging Classroom"*)

University-Wide GET SET Teaching Conference (certificate, October 19, 2013)

Assistance in Graduate Advising (with Prof. C.A. Shoemaker at Cornell University)

Haoyu Jia, Master of Engineering project, Computer Science, 02/2013 - 05/2013

Kyle Perline, summer project in uncertainty analysis, Applied Mathematics, 05/2013 - 08/2013

Min Pang, research project, Python implementations of Matlab codes, Environmental Engineering, 07/2013 - 07/2014

Professional Activities

Member of INFORMS (Institute of Operations Research and the Management Sciences)

Member of SIAM (Society for Industrial and Applied Mathematics)

Reviewer for (among others) *SIAM Journal on Optimization*, *INFORMS Journal on Computing*, *Computers & Operations Research*, *European Journal of Operational Research*, *Optimization - A Journal of Mathematical Programming and Operations Research*, *Journal of Global Optimization*, *Optimization & Engineering*, Reviewer for Winter Simulation Conference 2013

Honors, Awards, Achievements, Funding

Lab-wide LDRD recipient for the development of data-driven models to support decision making in groundwater management in California, USA

Early Career Development LDRD awardee to develop algorithms for computationally expensive black-box optimization under uncertainty, 10/2017-9/2019

Women @ The Lab award for outstanding achievements in the areas of science, technology, engineering, and mathematics, 11/2015

Luis W. Alvarez Postdoctoral Fellowship in Computing Sciences, Lawrence Berkeley National Laboratory, Lab Directed Research and Development & Advanced Scientific Computing Research funding, 08/2014 - 09/2017

Graduation Award in recognition of completing a doctoral degree at a young age, Industrial Research Fund at Tampere University of Technology, 800€, 06/2013

Finnish Academy of Science and Letters, Vilho, Yrjö and Kalle Väisälä Foundation Fellowship, 15000€ (in addition to regular Ph.D. student/researcher salary), 01/2011 - 03/2012

Graduate School position, 01/2010 - 12/2012
fully funded Ph.D. position in the **Tampere Doctoral Program in Information Science and Engineering (TISE)** for Ph.D. studies and research activities, covered salary and conference travels

Graduate School position, 09/2008 - 12/2009
fully funded Ph.D. position in **Tampere University of Technology's Graduate School** for Ph.D. studies and research activities, covered salary

Outreach, Volunteering for Berkeley Lab

Mentor in Early career training program in Computational research division, ongoing

Mentor in LBNL Computing Sciences Mentoring Program, ongoing

Guest speaker in LBNL's Computing Sciences Summer Student program, 07/2019

Guest speaker at Workforce Development & Education internship program, 06/2019

Panelist in BLEND program of Workforce Development & Education, June17, 2017

Guest speaker at Workforce Development & Education internship program, 05/2016

Chaperone for girl and boy scouts at Nuclear Science Day, 04/2016

Student mentor for Albany High School job shadow day, 04/2016, 04/2017

Tabling at annual Solano Avenue Stroll: providing information about the lab and handing out informational flyers, 09/2015

BLAZES instructor (Berkeley Lab Adventure Zone in Elementary Science), teaching 5th graders hands-on elementary science, 09/2015 - present, once per month

Computing Sciences Postdoc Group co-coordinator, seminar and social event organization, 10/2014 - 05/2017

Volunteer for WSEC Women Scientists and Engineering Council, 10/2015 - present

Publications

Papers in Refereed Journals

J. Müller, M. Day. *Surrogate optimization of computationally expensive black-box problems with hidden constraints*, 2019, INFORMS Journal on Computing, published online, `https://doi.org/10.1287/ijoc.2018.0864`

J. Müller. *An Algorithmic Framework for the Optimization of Computationally Expensive Bi-Fidelity Black-Box Problems*, 2019, INFOR: Information Systems and Operational Research, published online, `https://doi.org/10.1080/03155986.2019.1607810`

W. Langhans, **J. Müller**, W. Collins. *Optimization of the Eddy?Diffusivity/Mass?Flux shallow cumulus and boundary?layer parameterization using surrogate models*, 2019, Journal of Advances in Modeling Earth Systems, published online `https://doi.org/10.1029/2018MS001449`

O. Karslıoğlu, M. Gehlmann, **J. Müller**, S. Nemšák, J. Sethian, A. Kaduwela, H. Bluhm, C. Fadley. *An Efficient Algorithm for Automatic Structure Optimization in X-ray Standing-Wave Experiments*, 2018, Journal of Electron Spectroscopy and Related Phenomena, 230:10-20

G. Conti, S. Nemšák, C.-T. Kuo, M. Gehlmann, C. Conlon, A. Keqi, A. Rattanachata, O. Karslıoğlu, **J. Müller**, J. Sethian, H. Bluhm, J.E. Rault, J.P. Rueff, H. Fang, A. Javey, C.S. Fadley. *Characterization of free standing InAs quantum membranes by standing wave hard x-ray photoemission spectroscopy*, 2018, APL Materials, 6, 058101.

E. Lohrmann, Z. Lukić, D. Morozov, **J. Müller**. *Programmable In Situ System for Iterative Workflows*, 2017, Job Scheduling Strategies for Parallel Processing

J. Müller, J. Woodbury. *GOSAC: Global Optimization with Surrogate Approximation of Constraints*, 2017, Journal of Global Optimization, 69(1):117-136

J. Müller. *SOCEMO: Surrogate Optimization of Computationally Expensive Multi-Objective Problems*, 2017, INFORMS Journal on Computing, 29(4):581-783

J. Müller. *MISO: Mixed-Integer Surrogate Optimization Framework*, 2016, Springer Optimization and Engineering, 17 (1):177-203

J. Müller, R. Paudel, C.A. Shoemaker, J. Woodbury, Y. Wang, N. Mahowald. *CH4 Parameter Estimation in CLM4.5bgc Using Surrogate Global Optimization*, 2015, Geoscientific Model Development, 8 (10): 3285-3310

J. Müller, T. Krityakierne, C.A. Shoemaker. *SO-MODS: Optimization for High Dimensional Computationally Expensive Multi-Modal Functions with Surrogate Search*, 2014 IEEE Congress on Evolutionary Computation (CEC), July 6-11, 2014, Beijing, China, pages 1092-1099

J. Müller, C.A. Shoemaker. *Influence of Ensemble Surrogate Models and Sampling Strategy on the Solution Quality of Algorithms for Computationally Expensive Black-Box Global Optimization Problems*, 2014, Journal of Global Optimization, 60 (2):123-144

J. Müller, C.A. Shoemaker and R. Piché. *SO-I: A Surrogate Model Algorithm for Expensive Nonlinear Integer Programming Problems Including Global Optimization Applications*, 2013, Journal of Global Optimization, 59 (4): 865-889

J. Müller, J. Kanniainen and R. Piché. *Calibration of GARCH (generalized autoregressive conditional heteroskedasticity) Models Using Concurrent Accelerated Random Search*, 2013, Applied Mathematics and Computation, 221: 522-534

J. Müller, C.A. Shoemaker, and R. Piché. *SO-MI: A Surrogate Model Algorithm for Computationally Expensive Nonlinear Mixed-Integer Black-Box Global Optimization Problems*, 2013, Computers and Operations Research, 40 (5): 1383-1400

J. Müller and R. Piché. *Mixture Surrogate Models Based on Dempster-Shafer Theory for Global Optimization Problems*, 2011, Journal of Global Optimization, 51 (1): 79-104

J. Müller. *Approximative Solutions to the Bicriterion Vehicle Routing Problem with Time Windows*, 2010, European Journal of Operational Research, 202 (1): 223-231

Papers in Revision

T. Takhtaganov, Z. Lukić, **J. Müller**, D. Morozov. *Cosmic Inference: Constraining Parameters With Observations and Highly Limited Number of Simulations*

T Takhtaganov, **J. Müller**. *Adaptive Gaussian process surrogates for Bayesian inference*

J. Müller, J. Park, R.Sahu, C.Varadharajan, B. Arora, B. Faybishenko, D. Agarwal. *Surrogate Optimization of Deep Neural Networks for Groundwater Predictions*

O. Rouhani, **J. Müller**, C.A. Shoemaker, H.O. Gao *A Surrogate Optimization Algorithm for Solving Discrete Transportation Network Design Problems*

J. Müller, O. Rouhani, C.A. Shoemaker, H.O. Gao *Surrogate Model Optimization for Discrete Transportation Network Design Problems*

Conference Talks and Posters

SIAM Conference on Computational Science and Engineering (CSE19), February 25-March 1, 2019, session organizer

INFORMS Annual Meeting, November 4-7, 2018, Phoenix, AZ, USA, invited talk

2018 SIAM Annual Meeting, July 9-13, 2018, Portland, OR, USA, session organizer

2018 INFORMS Optimization Society Conference, March 23-March 25, 2018, Denver, CO, USA, invited talk

15th EUROPT Workshop on Advances in Continuous Optimization, July 12-14, 2017, Montreal, Canada, invited talk

2017 SIAM Conference on Computational Science and Engineering, February 27-March 3, 2017, Atlanta, GA, USA, invited talk

Seminar talk *Surrogate Models in Computationally Expensive Black-Box Simulation Optimization*, San Jose State University, CA, USA, February 9, 2017

2016 SIAM Annual Meeting, July 11-15, 2016, Boston, MA, USA, contributed talk, session chair

INFORMS International Meeting 2016, June 12-15, 2016, Hilton Waikoloa Village, HI, USA, contributed talk

CORS 58th Annual Conference, May 30-June 1, 2016, Banff, Alberta, Canada, contributed talk

Stanford-Berkeley Research Meetup 2016, May 1, 2016, Stanford, CA, USA, contributed talk

IMA Collaboration Workshop: Optimization and UQ in Energy and Industrial Applications, February 22-24, 2016, Minneapolis, MN, USA, invited talk

Bay Area Scientific Computing Day, December 11, 2015, Berkeley, CA, USA, invited talk

22nd International Symposium on Mathematical Programming (ISMP 2015), July 12-17, 2015, Pittsburgh, PA, USA, invited talk

CORS/INFORMS International Conference, June 14-17, 2015, Montréal, QC, Canada, invited talk

Invited seminar talk *Surrogate Model Optimization* at Carleton University, Department of Systems and Computer Engineering, Ottawa, Canada, June 11, 2015

SIAM Conference on Computational Science and Engineering, March 14-18, 2015, Salt Lake City, UT, USA, session co-organizer and chair

AGU Fall Meeting 2014, December 15-19, 2014, San Francisco, CA, USA, scientific poster

INFORMS Annual Meeting 2014, November 9-12, 2014, San Francisco, CA, USA, contributed talk and session chair

Berkeley Lab Computing Sciences Seminar, August 29, 2014, Berkeley, CA, USA

Mixed-Integer Nonlinear Programming, June 2-5, 2014, Carnegie Mellon University, Pittsburgh, PA, USA, scientific poster

4th New York Conference on Applied Mathematics, November 9, 2013, Cornell University, Ithaca, NY, USA, contributed talk and session chair

CESM (community earth system model) tutorial, August 12-16, 2013, Boulder, CO, USA, NCAR-funded participation

21st International Symposium on Mathematical Programming (ISMP 2012), August 19-24, 2012, Berlin, Germany, invited talk

Global Optimization Workshop 2012, June 26-29, 2012, Natal, Brazil, contributed talk

INFORMS Annual Meeting 2011, November 13-16, 2011, Charlotte, NC, USA, contributed talk

MOPTA 2011, August 17-19, 2011, Lehigh University, Bethlehem, PA, USA, contributed talk

Optimization 2011, July 24-27, 2011, Lisbon, Portugal, contributed talk

SIAM Conference on Optimization, May 16-19, 2011, Darmstadt, Germany, contributed talk

4th Nordic Optimization Symposium, September 30 - October 2, 2010, Aarhus, Denmark, contributed talk

SULATIS (Finnish Society of Computational Sciences), Computational Sciences Day, September 29, 2010, Kuopio, Finland, scientific poster

Published Open-Source Optimization Codes

SHEBO: surrogate model optimization algorithm for computationally expensive, black-box global optimization problems with hidden constraints.

MATSuMoTo: The MATLAB Surrogate Model Toolbox for Computationally Expensive Black-Box Global Optimization Problems, arXiv: 1404.4261, April 2014

MISO Mixed Integer Surrogate Optimization framework (MATLAB)

Implementations of Stochastic Radial Basis Function Algorithm for Global Optimization (MATLAB and Python 2.7)

Implementations of DYCORS Algorithm for Global Optimization (MATLAB and Python 2.7)